PCCP themed collection: High performance computing in the chemistry of materials

Guest Editors: Richard Catlow and Scott Woodley (University College London)

PCCP is delighted to announce the high-profile themed web collection on ‘High performance computing in the chemistry of materials’. It is our pleasure to invite you to submit an original research article for this collection.

Accepted articles will be published in Physical Chemistry Chemical Physics (PCCP) as and when they are ready, with a web collection prepared in 2014. The collection will receive good exposure, and get significant promotion.

PCCP is a high-impact, community spanning, international journal publishing work of the highest quality in the broad fields of physical chemistry, chemical physics and biophysical chemistry.

Deadline for Submissions: 17th March 2014

The applications of high performance computing (HPC) now play a major role in almost all areas of chemistry, but they are particularly effective in the field of materials chemistry. HPC is now being used in an increasingly predictive manner in modelling the structures (both surface and bulk), properties and reactivity of materials; and modelling techniques are now widely used in a complementary manner with experiments.

The collection will highlight the current state-of-the-art in the field by focussing on the following applications areas:

- Energy materials
- Surface Structures and properties
- Reactivity and catalysis
- Nano- and defect Chemistry
- Biomaterials
- Electronic materials
- Soft Matter and porous materials

Manuscripts can be submitted in any reasonable format using our online submissions service. Submissions should be high quality manuscripts and will be subject to rigorous peer review. Please indicate upon submission that your manuscript is intended for this themed collection.

The deadline for submissions to the collection is 17th March 2014, though submissions before this date are of course welcomed.